Notes for convert.f90, the Fortran program generating hot CO2 IR line list using AI-3000K data files (01/10/2023)

Use convertLS.f90 to generate line shape parameters along with the line list in HITRAN format

[Prepared for "AI-3000K Infrared Line List for Hot CO2"; contact xhuang@seti.org for questions]

0. Compile the convert.f90 into convert.x, e.g. ifort convert.f90 -o convert.x -mcmodel=large

1. All the files under “code.and.files” should be put under the same working directory. Please decompress the 4 co2.xxx.levels....tgz files first.

2. Select the compressed .tgz files for the range of IR simulation. They are stored in 10 cm-1 bins. Filenames are fort.7000.1xxxx.tgz:
...10001.tgz - 0 - 10 cm-1
...10002.tgz - 10-20 cm-1
...10003.tgz - 20-30 cm-1
…
... 10500.tgz - 4990 - 5000 cm-1
…
… 11000.tgz - 9990 - 10000 cm-1
…
… 11999.tgz - 19980 - 19990 cm-1
…12000.tgz - 19990 - 20000 cm-1
Put the selected .tgz file(s) under the same working directory of the convert.x and the decompressed co2.xxx.levels… and the zpe+part file.

3. Run ./convert.x, it will decompress and convert the fort.7000.xxxxx.tgz files, one by one, into their corresponding list file: co2list.zzzzzcm-1. e.g. fort.7000.11234tgz → co2list.12340cm-1. The convert.f90 is customizable, see below.

4. The line list output format can be adjusted as you need. In convert.f90, lines #151 - #163 explain the data choices

```
! Please choose your own format to write out whatever quantities that fit your needs
! so here is just an example for full length, i.e. including everything I can think of
! iso-isotopologue #, 21-24 for 626/636/628/627
! om2 - transition wavenumber
! a21 - Einstein A21
! si(0:5)*ab(is) - 100% line intensities at user-specified and 5 pre-set temperatures are scaled by their terrestial abundances
! jf, iparf, irf - J, parity, root number for E'
! ji, ipari, iri - J, parity, root number for E"
! jw(1:5) - importance indicator for 5 pre-set temperatures, 0 - to ignore, 1 - to include
! ef, ei - E' and E"
! ie(:,:,:,:,1:3) are the v1v2v3 from vtet, ie(:,:,:,:,6:13) are the p (polyad #),c (wang's sym),n(root# in that polyad) and v1v2l2v3r from CDSD
! if you need wang's symmetry:  mod(j+ipar,2)=0 --> e;  mod(j+ipar,2)=1 --> f
! now the first intensity value after A21 is for the temperature user specified at line #45.

  write(7001,1213)iso,om2,a21,si(0:5)*ab(is),jf,iparf,irf,ji,ipari,iri,jw(1:5), &
             ef,ei,ie(is,jf,iparf,irf,1:3),ie(is,jf,iparf,irf,6:13),ie(is,ji,ipari,iri,1:3),ie(is,ji,ipari,iri,6:13)
1213    format(i2,f12.5,7es12.5,i4,i2,i6,i4,i2,i6,5i2,2f12.5,3i3,1x,2i3,i5,5i3,2x,3i3,1x,2i3,i5,5i3)
```

`A line example is below, note the energies in this example were X01d-PES based, not replaced by CDSD2019 energies yet.`

```
22  4999.99970 2.06453E-03 2.30683E-37 2.19914E-45 5.84959E-32 6.98025E-30 1.42623E-29 1.27300E-29  83 1   399  82 2    84 0 1 1 1 1
14713.00637  9713.00667  2 14  0  17  1 -119  7  3  3  0  1    2  3  2  10  1  -35  2  0  0  2  2
```

From '0 1 1 1 1', we can tell this 636 R82 hot band transition is part of 1000K, 2000K, 3000K and 4000K lists, but not for 296K list. Note the first intensity after A21 is at user provided temperature (*T* = 500K here), see #7 below. Its intensity at 2000K is 6.98025E-30 cm/molecule. Terrestrial abundance included in all 6 intensities. E'=14713.10314 cm-1, E"=9713.06930 cm-1, Ames VTET vib quantum numbers are: (v1v2v3)' = 2v1+14v2, (v1v2v3)"= 2v2+3v2+2v3, 399th root of 83e block ← 84th root of 82e block. The CDSD2019 assignment is: 73301e ← 20022e, 119th root of P17 ← 35th root of P10. The minus sign of "-119" and "-35" means the match is probably reliable.

Note: the CDSD2019 levels are available up to 24,000 cm-1 and J=150. AI-3000K list has J up to 250 (200) and E' up to 40,000 (36,000) cm-1 for 626 (636, 628, 627).

Example: to write out om2, A21, E", J' and Ames vtet based vib quanta differences v1v2v3' - v1v2v3" -- we know sometimes it could be badly off

```
        write(7001,1213)om2,a21*ab(is),ei,jf,ie(is,jf,iparf,irf,1:3)-ie(is,ji,ipari,iri,1:3)
1213    format(f12.5,es12.5,f12.5,i4,3i3)
```

5. Convert.f90 lines #99-#117, explain the two sets of line positions: Ames X01d PES based vs. CDSD2019 replaced. This is a 1-to-1 replacement.

```
! You can choose Ames-X01d PES based energies OR CDSD energies (when available, J=0-150, 0-24000 cm-1)
! the .tgz data were sorted by Ames-X01d based wavenumbers. You may re-sort them after using CDSD energies.
! to use Ames original:
! ef=e(is,jf,iparf,irf,1); ei=e(is,ji,ipari,iri,1)
! by default to use CDSD levels when available + Ames original for remains
  ef=e(is,jf,iparf,irf,1)+e(is,jf,iparf,irf,3)
  ei=e(is,ji,ipari,iri,1)+e(is,ji,ipari,iri,3)

! 2021-04-13 update: We tried to match part of X01d-PES levels with CDSD2019 (J<150, E'<15,000 cm-1)
!     if the 8th parameter in the ie() array was set to negative, which indicates the match was probably reliable (no guarantee though)
!     It is interesting to find out how much impact the inevitable inconsistency caused by such replacements will have at certain temperature
!   for high-T test, suggest to start with CDSD energy replacement for ALL J<=150 and E<15000 cm-1 levels.
!   if runs into some problems, we can enforce the filter below, i.e. to use the ie(,8)<0 & E<15000 cm-1 filter.
!   for potential fixes, we just need to update the energy level list files in future.
!   but for now, not sure how much difference they will make
        !if(ie(is,jf,iparf,irf,8).gt.0)ef=e(is,jf,iparf,irf,1)
  !if(ie(is,ji,ipari,iri,8).gt.0)ei=e(is,ji,ipari,iri,1)
        !if(ef.gt.15000.d0)ef=e(is,jf,iparf,irf,1)
        !if(ei.gt.15000.d0)ei=e(is,ji,ipari,iri,1)
```

6. Convert.f90 lines #119-#121, this serves as the filters on isotopologue & E' / E" thresholds. 'ef' / 'ei' for E' / E" in cm-1.

```
! Your E' cutoff for co2 626 (and other iso) can be put here, I suggest to try E'=37500 cm-1 and E=40000 cm-1
!       if(is.eq.1.and.ef.gt.36000.d0)goto 301
! by default it will go up to 40,000 cm-1 for 626.  (other 3 isos always up to 36000 cm-1)
```

7. How to generate a line list at user-specified temperature, other than 296K, 1000K, 2000K, 3000K, or 4000K.

User can specify a target temperature at line #45, as t(0). Accordingly, the partition function values of 4 isos are computed at line #54, and write out in line #58. The intensity at t(0) is computed from line #134 to line #140, saved as si(0), then output by line #163 - #165.

The convert.f90 is updated (old version saved as convert.f90.20210415). The screenshot on page 1 of this google.doc is also updated.

8. calculate the total number of lines for whole list generation vs for each 10 cm-1

Current convert.f90 has “nab=0” at line #66, for #lines in each 10 cm-1.

If one needs to get the total number of lines from each isotopologue in a wide (or full) range line list generation, the nab(4) should be defined as integer*8, and do not reset nab=0 for each .tgz list file.

Supplementary file for “AI-3000K Infrared Line List for Hot CO2”

prepared by Xinchuan Huang, on 01/2023

Notes for AI-3000K (05/2022 version) line list calculation and additional statistics.

Compared to preliminary 2021 versions, this latest 2022.May list has following updates or differences :

1. The intensity calculation now has built-in *P/R* consistency, no more need for Cs-sym intensity calc (and match) on 626 and 636. All 4 isotopologues have more self-consistent intensities computed.
2. Because the experiment validation and list comparisons are up to 3000K, and our analysis indicates the 4000K convergence probably requires more robust PES/DMS at higher energies (i.e., >40,000 cm-1):
   A. In the first step of individual isotopologue line list calculations (writing out base list), for every 0.01 cm-1 interval, we adopted 99.99% for 296K and 1000K, 99.95% for 2000K, and 99.9% for 3000K and 4000K. In the 2nd step (generate lists for iso-mix) line list size reduction for every 0.01 cm-1 interval, we adopted the same thresholds: 99.99% for 296K and 1000K, 99.95% for 2000K, and 99.9% for 3000K and 4000K.
   Note that for 626, we run 0-36,000 cm-1 and 0-40,000 cm-1 intensity tests together, the S_min threshold selected for each 0.01 cm-1 interval ensures the sum of intensity is converged for both ranges. In most (but not all) cases, S_min(40K) < = S_min(36K).
   B. In the iso-mixing step, we still use 99% for the intensity_sum threshold at 4000K, but raise the 2000K threshold from 99.9% to 99.95%, and raise the 3000K threshold from 99% to 99.9%. As a result, the data size of the 2022.5 final list is effectively doubled. Now the 2000 .tgz files occupy ~400GB.
3. More conservative cutoffs were applied during the stage of identifying fake intensity, finding related upper levels, and rejecting all other transitions associated with those levels. Very small intensity reductions can be found near 20,000 cm-1 at 3000K. No other differences were found at lower temperature or lower wavenumber range. Numerically equivalent (but not identical) to the 2021 list, especially below 10,000 cm-1.

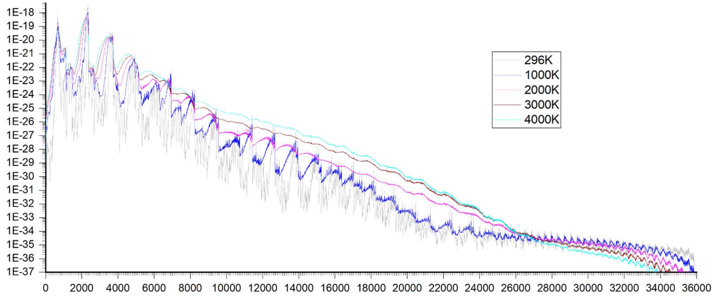
Statistics and Notes:

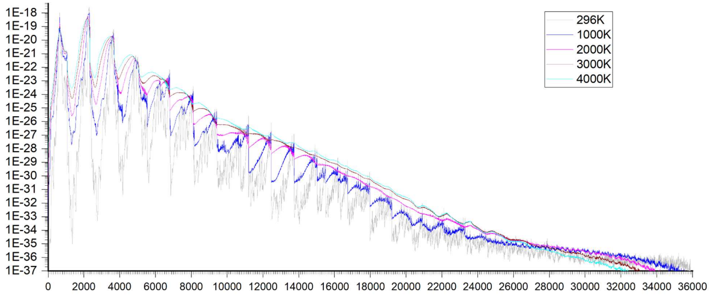
1. The 2021 version of convert.f90 works fine. The v5 version of energy level lists are almost numerically identical to the v4 version. Should not cause any discernible differences in simulation or analysis.
2. Number of transitions: (628 becomes more significant than 636 at higher temperature and higher wavenumber)

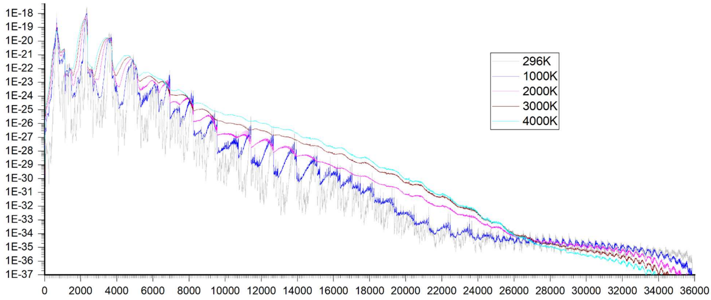
	626	636	628	627	Sum
296K	8679292	4102781	9187117	5896321	
1000K	574267343	129459222	208009376	94383807	
2000K	11581289410	1259622929	2252742848	717929106	
3000K	27397362378	2691372006	4578190786	1294391142	
4000K	16955873906	815640117	1041707073	203707345	

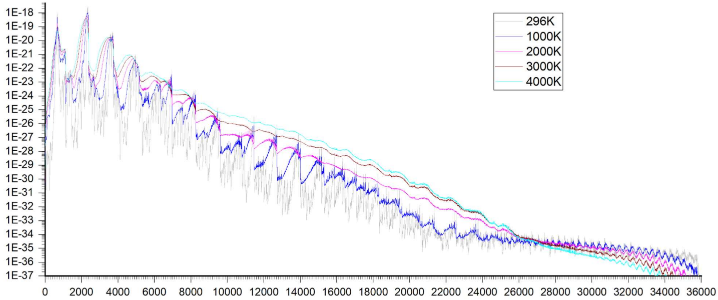
Total 27548493437 +2780854018 +4801316888 +1418062103 = 36,548,726,446 lines

3. Overview of the AI-3000K line lists for the 4 isotopologues, in the order of 626, 636, 628, and 627

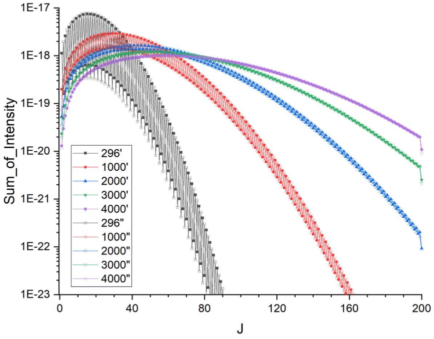




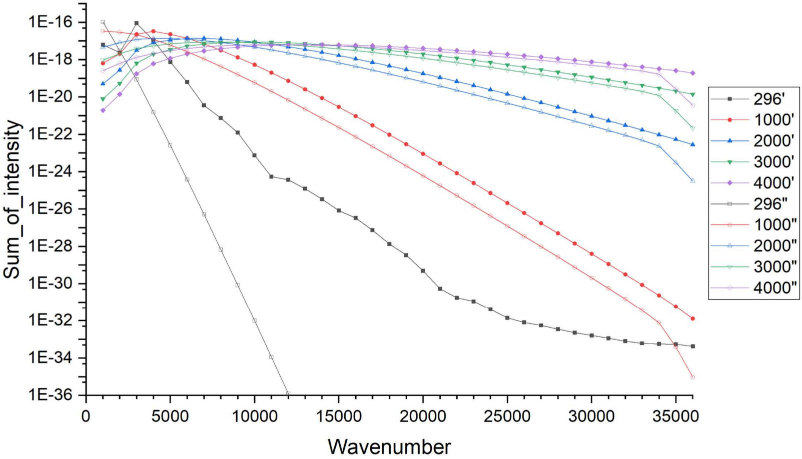




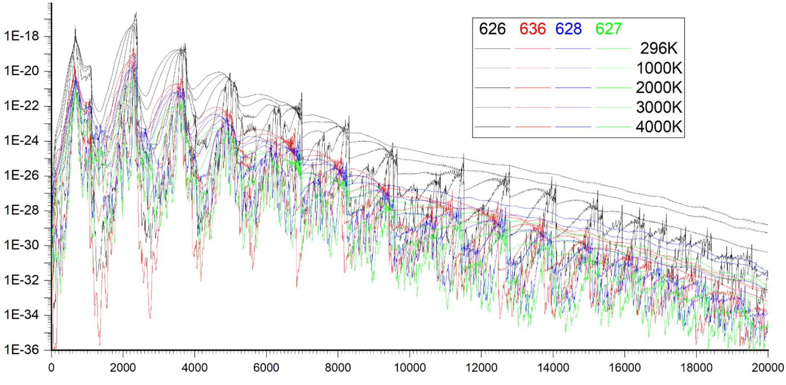
4. CO2 636 list sanity check, the intensity distribution along J’ and J”



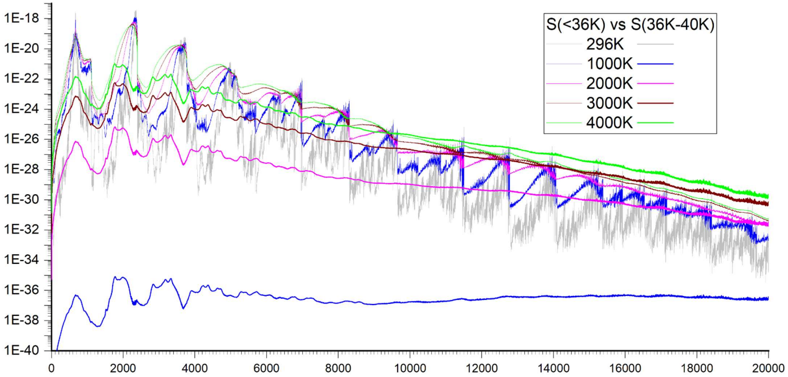
CO2 636 sanity check, the intensity associated with upper state energy and lower state energy:



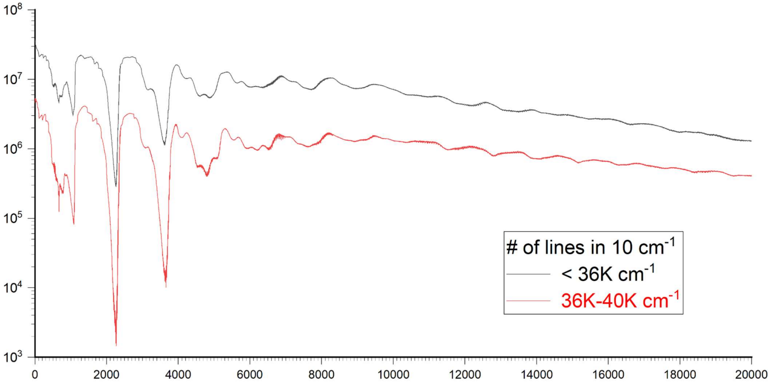
5. Isotopologue contributions to the final iso-mixed line list at 5 temperatures:



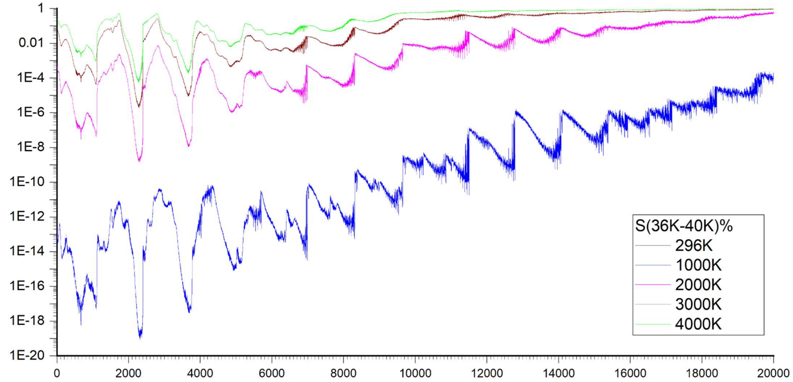
6. In final list, <36K cm-1 vs 36K-40K cm-1, statistics by 1 cm-1 : (a) associated intensities

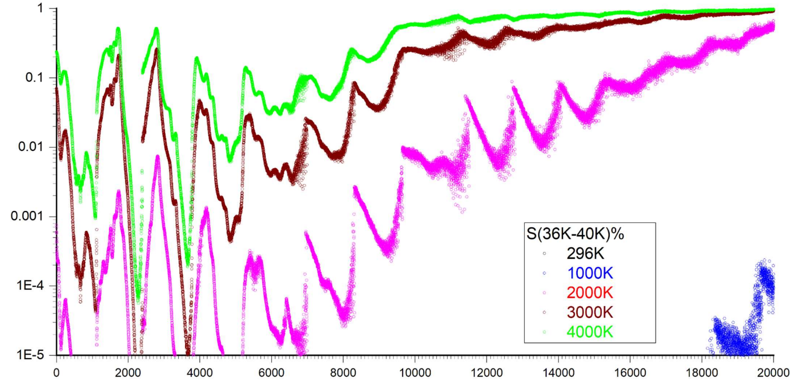


(b) associated number of lines

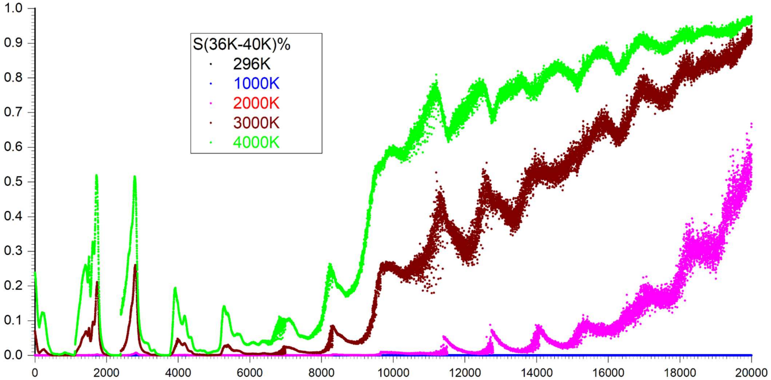


(c) the intensity ratio in total intensity sum = S(<36K) + S(36K-40K)

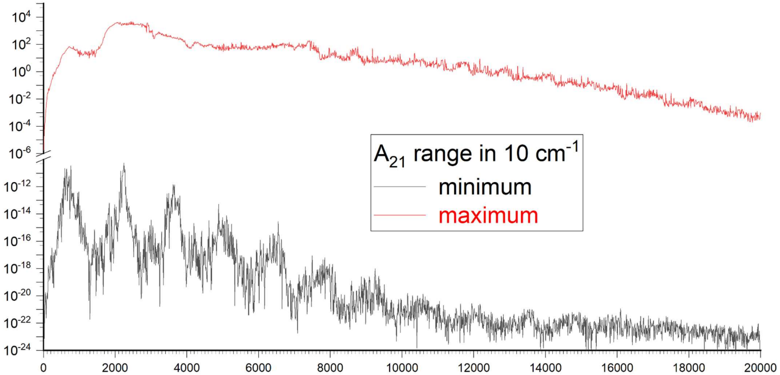

1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
1E-14
1E-16
1E-18
1E-20
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
S(36K-40K)%
296K
1000K
2000K
3000K
4000K


1
0.1
0.01
0.001
1E-4
1E-5
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
S(36K-40K)%
296K
1000K
2000K
3000K
4000K

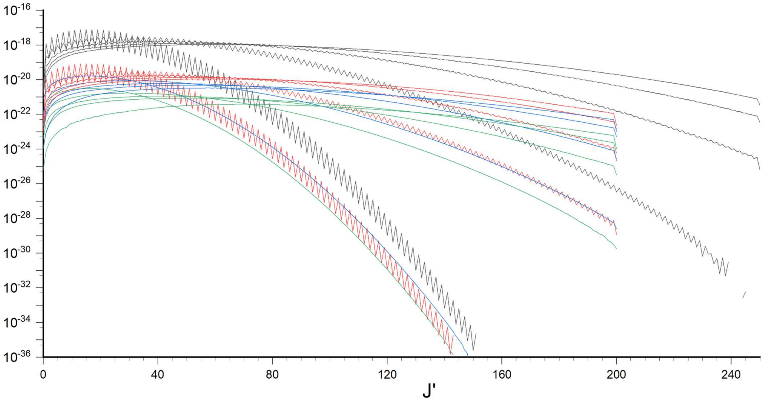
or



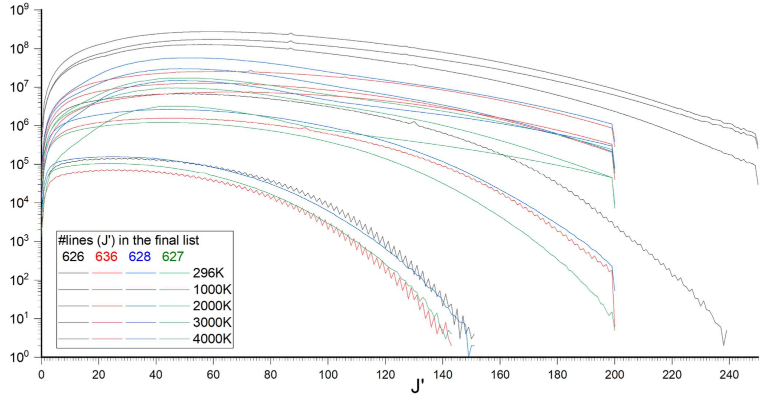
7. In final list, the range of A21 coefficients in each 10 cm-1



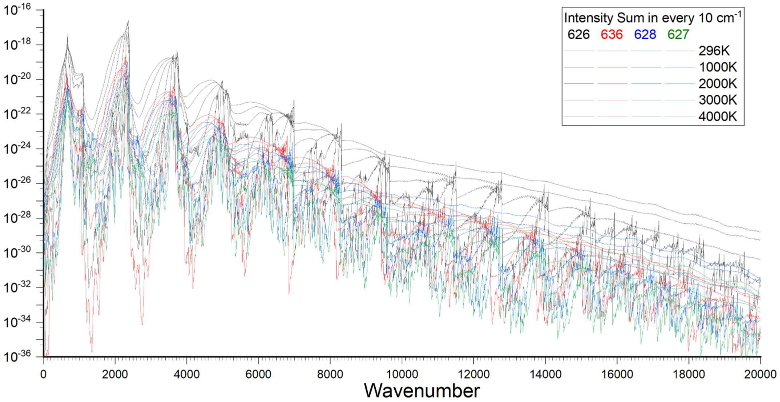
8. In final list, the intensity distribution along J' [626 black, 636 red, 628 blue, 627 olive/green]



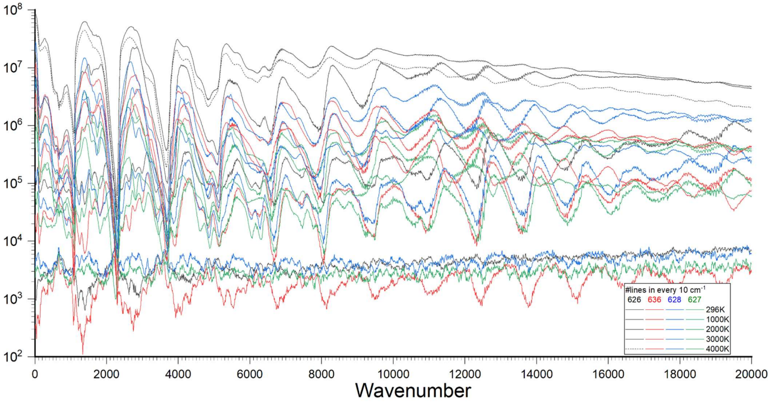
The number of lines distribution along J' – We see small bumps at a few J's, which are iso & temperature dependent, but we do not know how much irregular intensities are there, or if they did cause any detectable noises.



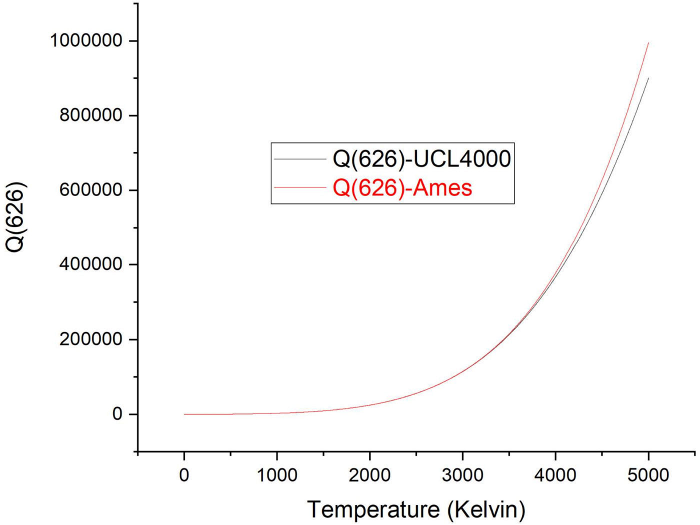
9. In final list, the intensity sum of each isotopologue in 10 cm-1 interval, same plot as #5.



The number of isotopologue lines in each 10cm-1 interval. Note the 2nd highest black (626) curve below 10000 cm-1 is the short-dashed line for the 4000K list, which is less than the 3000K list (the highest curve), due to the 99% intensity cutoff we adopted for 4000K.



—----------Above was prepared on 05/18/2022—--------



Partition function comparison plot is added on 09/01/2022